

ABSTRACT OF THE DISCLOSURE

A method in a data processing system for generating and storing in a database at least one descriptor vector and at least one reference frame for at least one region of a molecule includes a step of generating an entry including: i) a key derived from the at least one descriptor vector, wherein the key identifies the at least one region, and ii) a set of axes derived from property distribution information of the at least one region, the set of axes characterizing the at least one region. The method further includes steps of applying a mapping to the descriptor vector associated with the at least one region based on preselected criteria and storing the entry in a memory, wherein the key is associated with the entry such that the key indexes the entry for retrieval thereof.